



Study of the footprints of short-term variation in XCO₂ observed by TCCON sites using NIES and FLEXPART atmospheric transport models

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Abstract. The Total Carbon Column Observing Network (TCCON) is a network of ground-based Fourier transform spectrometers (FTSs) that record near-infrared (NIR) spectra of the sun. From these spectra, accurate and precise observations of CO₂ column-averaged dry-air mole fractions (denoted XCO₂) are retrieved. TCCON FTS observations have previously been used to validate satellite estimations of XCO₂; however, our knowledge of the short-term spatial and temporal variations in XCO₂ surrounding the TCCON sites is limited.

In this work, we use the National Institute for Environmental Studies (NIES) Eulerian three-dimensional transport model and the FLEXPART (FLEXible PARTicle dispersion model) Lagrangian particle dispersion model (LPDM) to determine the footprints of short-term variations in XCO₂ observed by operational, past, future and possible TCCON sites. We propose a footprint-based method for the collocation of satellite and TCCON XCO₂ observations and estimate the performance of the method using the NIES model and five GOSAT (Greenhouse Gases Observing Satellite) XCO₂ product data sets. Comparison of the proposed ap-

proach with a standard geographic method shows a higher number of collocation points and an average bias reduction up to 0.15 ppm for a subset of 16 stations for the period from January 2010 to January 2014. Case studies of the Darwin and Reunion Island sites reveal that when the footprint area is rather curved, non-uniform and significantly different from a geographical rectangular area, the differences between these approaches are more noticeable. This emphasises that the collocation is sensitive to local meteorological conditions and flux distributions.

1 Introduction

Satellite observations of the column-averaged dry-air mole fraction of CO₂ (XCO₂) have the potential to significantly advance our knowledge of carbon dioxide (CO₂) distributions globally and provide new information on regional CO₂ sources and sinks. Observations of XCO₂ are available from space-based instruments such as the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY; data available for the period 2002–2012; Bovensmann et al., 1999), the Greenhouse Gases Observing Satellite (GOSAT; data available since 2009; Kuze et al., 2009, 2016; Yokota et al., 2009) and the Orbiting Carbon Observatory-2 (OCO-2; available since the middle of 2014; Crisp et al., 2004). These satellites provide unprecedented spatial coverage of the variability in XCO₂ around the world, with the exception of polar regions and areas with dense clouds. These observations are, however, limited by the orbit of the satellites, which typically measure in the local afternoon.

Ground-based Fourier transform spectrometer (FTS) observations available from the Total Carbon Column Observing Network (TCCON) (Deutscher et al., 2010; Geibel et al., 2010; Messerschmidt et al., 2010, 2012; Ohyama et al., 2009; Washenfelder et al., 2006; Wunch et al., 2011, 2015) provide dense temporal resolution and are more precise and accurate than space-based instruments. However, the number of ground-based FTS sites is limited, with just 23 operational sites and several approved for the future. These sites are sparsely distributed, and Siberia, Africa, South America and the oceans from middle to high latitudes are poorly covered. Despite this limitation, FTS observations are used to validate satellite retrievals in order to assess bias, variability and other key parameters (e.g. Wunch et al., 2011; Lindqvist et al., 2015).

The spatial and temporal coverage of satellite observations over TCCON sites is sparse in space and time due to cloud and aerosol filters, retrieval selection criteria and post-retrieval data quality filters. To obtain satellite observation data at the location and time of interest it is necessary to apply a collocation method for aggregating neighbouring soundings. All collocation methodologies implement inter-

polation techniques. It is important to minimise the interpolation errors, which cause an uncertainty that is incorporated into the variability of the colocated/validation data comparison (Nguyen et al., 2014). Currently available methods for XCO₂ collocation include geographical (e.g. Cogan et al., 2012; Inoue et al., 2013; Reuter et al., 2013), T700 (it implies that the air with the same history of transport derived from the 700 hPa potential temperature has the same XCO₂; Wunch et al., 2011), model-based (Guerlet et al., 2013) and geostatistical approaches (Nguyen et al., 2014).

In the geographical collocation method a spatial region around a TCCON site is selected together with a temporal window for selecting the satellite data. Inoue et al. (2013) used daily mean observations within a 10° × 10° area, Reuter et al. (2013) selected the monthly median of all observations within a 10° × 10° area, and Cogan et al. (2012) implemented narrower limits, using a 2 h mean period within a ±5° × ±5° area.

To increase the number of soundings, the spatial region may be expanded and additional selection criteria imposed. In the T700 collocation method proposed by Wunch et al. (2011), all observations within ±30° longitude, ±10° latitude, and ±2 K of the selected TCCON location and within ±5 days window are employed.

The model-based method proposed by Oshchepkov et al. (2012) and improved by Guerlet et al. (2013) uses daily mean values within 0.5 ppm of the 3-day-averaged model XCO₂ values and is located within ±25° longitude and ±7.5° latitude of a TCCON site.

Nguyen et al. (2014) developed a geostatistical collocation methodology that selects observations using a “distance” function, which is a modified Euclidian distance in terms of latitude, longitude, time and mid-tropospheric temperature at 700 hPa.

The majority of collocation methods described above have a common disadvantage; i.e. they work with a rectangular spatial domain, which is convenient for technical handling but does not reflect the impact of surface sources or sinks of CO₂ and the local meteorology in the area of interest. The spatial domains in collocations should take into account these features to ensure that only appropriate observations are selected. Keppel-Aleks et al. (2011, 2012) showed that the largest gradient in XCO₂ is formed mainly by the north–south flux distribution, with variations in XCO₂ caused mainly by large-scale advection. TCCON and satellite XCO₂ observations have pronounced temporal variability and are thus important in studies of short-term variations in XCO₂.

In this paper we study short-term variations in XCO₂ observed at TCCON sites. Although the XCO₂ is derived from column-averaged concentrations of CO₂, XCO₂ observations are most sensitive to near-surface fluxes. The XCO₂ variations are thus related to changes in the CO₂ mole fraction occurring near the surface surrounding the TCCON sites (hereafter known as the footprints of the TCCON sites).

The remainder of this paper is organised as follows: an overview of the method for estimating the footprints of TCCON sites is presented in Sect. 2. The results of the footprint estimation and a new method for collocation are presented and discussed in Sects. 3 and 4, and the conclusions are given in Sect. 5.

2 Method

To estimate the footprints of TCCON sites we used forward simulations employing the NIES Eulerian three-dimensional transport model (TM) and backward trajectory tracking using the FLEXPART LPDM model.

The key features of the NIES TM are as follows: a reduced horizontal latitude–longitude grid with a spatial resolution of $2.5^\circ \times 2.5^\circ$ near the equator (Belikov et al., 2011), a vertical flexible hybrid sigma–isentropic (σ – θ) grid with 32 levels up to the level of 5 hPa (Belikov et al., 2013b), separate parameterisation of the turbulent diffusivity in the PBL and free troposphere (provided by the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA-Interim reanalysis) and a modified Kuo-type parameterisation scheme for cumulus convection (Belikov et al., 2013a).

The NIES model has previously been used to study the seasonal and interannual variability in CO₂. Belikov et al. (2013b) reported that the NIES model is able to successfully reproduce the vertical profile of CO₂ as well as the seasonal and interannual variability in XCO₂. A comparison of modelled output with TCCON observations (Belikov et al., 2013b) revealed model biases of $\pm 0.2\%$ for XCO₂; on this basis we assume that the NIES TM is able to successfully reproduce the vertical profile of CO₂ at the locations of TCCON sites.

Firstly we run NIES TM for the target period (January 2010–February 2011) using 10 year's spin-up to ensure reduction of initialization errors. Then NIES TM CO₂ concentrations sampled at the location of TCCON sites at the level of 1 km above ground at 13:00 local time were used to initialise backward tracer simulations with the FLEXPART model.

FLEXPART is used to identify the source–receptor relationship of the CO₂ tracer. The CO₂ emission is the “source”, and the TCCON site is the “receptor”. Like other Lagrangian particle dispersion models (LPDMs), FLEXPART approximates a plume of atmospheric tracer by a cloud of particles. An efficient way of calculating sensitivity at the receptor is by solving the adjoint equation of tracer transport, which requires backward transport (Hourdin and Talagrand, 2006). Lagrangian models provide a efficient tool for backward transport modelling of a compact plume of particles, one plume representing a single observation. By tracking the pathway of each individual particle back in time and counting the particle residence times in the mixed layer at each grid cell the sensitivity coefficient or the footprint can be obtained

(Stohl et al., 2009). The sensitivity S of CO₂ concentration C to emissions F is the ratio of the change in C to an incremental change of F : $S = \partial C / \partial F$. Surface emissions change the concentration in the surface layer, while FLEXPART sensitivity to concentration in a surface grid cell at a given time is given by the number of particles that reside in the each surface grid cell divided by the total number of particles released.

The level of 1 km above ground typically corresponds to the top of the daytime planetary boundary layer (PBL). The PBL is the lowest part of the atmosphere and its behaviour is directly influenced by its contact with the planetary surface. Turbulence causes intensive vertical mixing of the air within the PBL, so CO₂ released from the surface is roughly uniformly distributed throughout the column of air in the PBL at local noon, when the maximum extent of vertical mixing occurs. The selected sampling time is also favourable for minimising errors in the initial CO₂ concentration calculated by NIES TM, as this type of chemical transport model has proved to be successful in resolving the diurnal vertical profiles of tracers (Belikov et al., 2013a).

To run the NIES TM and FLEXPART models we use fluxes obtained with the GELCA-EOF (Global Eulerian–Lagrangian Coupled Atmospheric model with Empirical Orthogonal Function) inverse modelling scheme (Zhuravlev et al., 2013). A priori fluxes consist of four types:

1. the Open-source Data Inventory of Anthropogenic CO₂ (ODIAC) (Oda et al., 2011) and the Carbon Dioxide Information Analysis Center's (CDIAC) (Andres et al., 2011) anthropogenic fluxes;
2. the Vegetation Integrative Simulator for Trace gases (VISIT) (Ito, 2010) biosphere fluxes;
3. the offline Ocean Tracer Transport Model (OTTM) (Valsala et al., 2013) oceanic fluxes;
4. the Global Fire Emissions Database (GFED) (Van der Werf et al., 2010) biomass burning emissions. Both models are driven by the Japanese Meteorological Agency Climate Data Assimilation System (JCDAS) data sets (Onogi et al., 2007).

Variations in TCCON XCO₂ are influenced by a large-scale processes. Keppel-Aleks et al. (2012) presented a robust relationship between weekly and monthly aggregated total column CO₂ and local net ecosystem exchange, while column drawdown has only a weak correlation with the regional flux on daily timescales. Thus the maximum trajectory duration for the FLEXPART was, therefore, set to 1 week. The FLEXPART model was run with resolution of 1° and 2 h time step for a 14-month period from January 2010 to February 2011.

Table 1. Details of operational TCCON sites.

Number	Site	Latitude (degrees)	Longitude (degrees)	Altitude (km)
1	Anmyeondo, Korea	36.54	126.33	0.03
2	Ascension Island	7.92	−14.33	0.03
3	Bialystok, Poland	53.23	23.03	0.18
4	Bremen, Germany	53.10	8.85	0.03
5	Caltech, USA	34.14	−118.13	0.23
6	Darwin, Australia	−12.42	130.89	0.03
7	Edwards, USA	34.96	−117.88	0.70
8	Eureka, Canada	80.05	−86.42	0.61
9	Garmisch, Germany	47.48	11.06	0.74
10	Izaña, Tenerife	28.30	−16.50	2.37
11	Karlsruhe, Germany	49.10	8.44	0.12
12	Lamont, USA	36.60	−97.49	0.32
13	Lauder, New Zealand	−45.04	169.68	0.37
14	Ny Ålesund, Spitsbergen	78.90	11.90	0.02
15	Orléans, France	47.97	2.11	0.13
16	Park Falls, USA	45.95	−90.27	0.44
17	Paris, France	48.85	2.32	0.10
18	Reunion Island, France	−20.90	55.49	0.09
19	Rikubetsu, Japan	43.46	143.77	0.36
20	Saga, Japan	33.24	130.29	0.01
21	Sodankylä, Finland	67.37	26.63	0.19
22	Tsukuba, Japan	36.05	140.12	0.03
23	Wollongong, Australia	−34.41	150.88	0.03

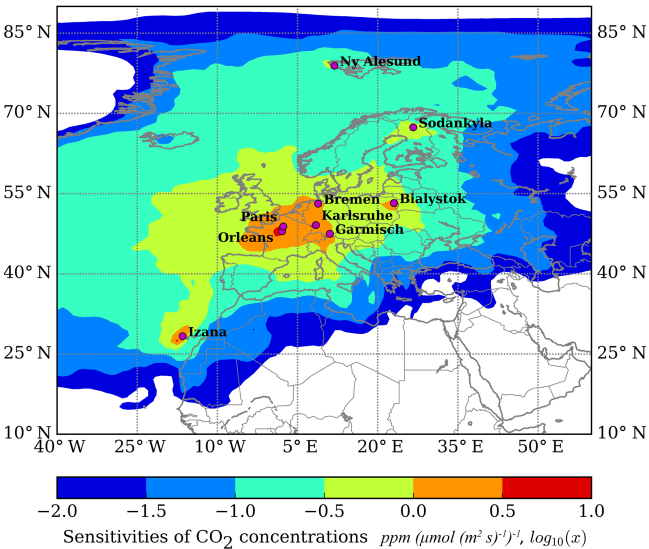


Figure 2. Distribution of the sensitivity of CO₂ concentrations ($\text{ppm}(\mu\text{mol}(\text{m}^2\text{s})^{-1})^{-1}$) in Europe with respect to the concentrations in adjacent cells, calculated using the FLEXPART model with a resolution of 1.0° for TCCON operational sites within Europe, using a tracer simulation initialised at the level of 1000 m.

Table 2. Past, future and possible TCCON sites.

Number	Site	Latitude (degrees)	Longitude (degrees)	Altitude (km)
1	Arrival Heights, Antarctica	−77.83	166.66	0.25
2	Burgos, Philippines	18.50	120.85	0.10
3	East Trout Lake, Canada	54.35	−104.98	0.49
4	Four Corners, USA	36.80	−108.48	1.64
5	Manaus, Brazil	−3.10	−60.02	0.09
6	Oxfordshire, UK	51.57	−1.32	0.07
7	Paramaribo, Suriname	5.80	−55.20	0.05
8	Poker Flat, USA	65.12	−147.47	0.21
9	Yekaterinburg, Russia	57.04	59.55	0.30

3 Results

3.1 Sensitivity of TCCON site footprints

We analysed two groups of TCCON sites: operational sites (Table 1; Figs. 1 and 2) and past, future and possible sites (Table 2; Fig. 3). We included Arrival Heights (Antarctica) and Yekaterinburg (Russia) in the second group, though the status of these monitoring stations is unclear. The footprint estimation is restricted to the summer season for high-latitude sites (Arrival Heights, Eureka, Ny Ålesund, Poker Flat and Sodankylä), due to limitations relating to the solar zenith angle.

3.1.1 Operational sites

North America

The five active American sites are located in the US and Canada, so they are sensitive to the western and central parts

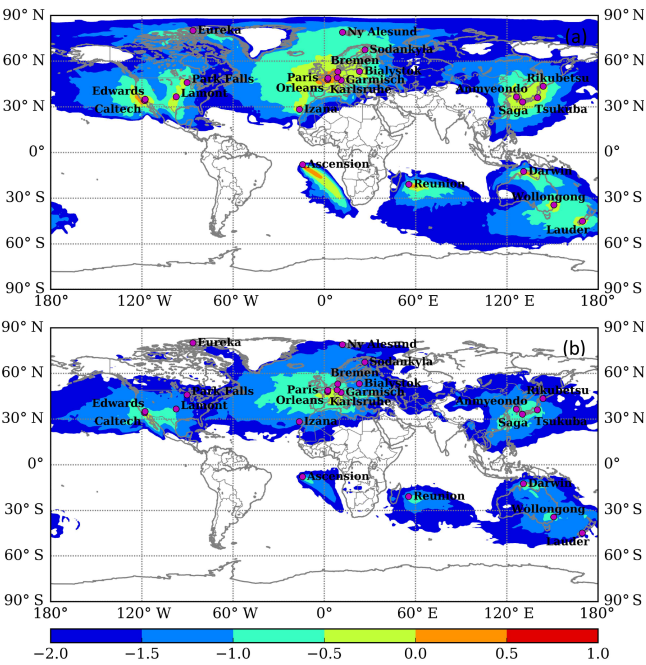


Figure 1. Global distribution of the sensitivity of CO₂ concentrations ($\text{ppm}(\mu\text{mol}(\text{m}^2\text{s})^{-1})^{-1}$) with respect to the concentrations in adjacent cells, calculated using the FLEXPART model with a resolution of 1.0° for the 23 TCCON operational sites: (a) tracer simulation initialised at the level of 1000 m, (b) tracer simulation initialised at the level of 3000 m that corresponds to 700 hPa based on the International Standard Atmosphere for dry air.

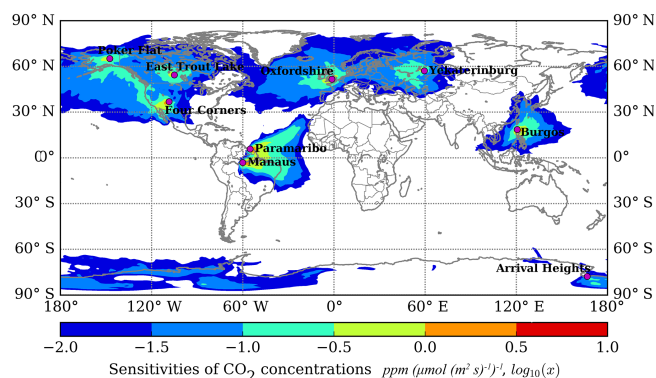


Figure 3. Global distribution of the sensitivity of CO₂ concentrations ($\text{ppm} (\mu\text{mol} (\text{m}^2 \text{s})^{-1})^{-1}$) with respect to the concentrations in adjacent cells, calculated using the FLEXPART model with a resolution of 1.0° for 9 past, future and possible TCCON operational sites, using a tracer simulation initialised at the level of 1000 m.

of North America, the northern part of Canada and Greenland and the eastern part of the Pacific Ocean. There are no TCCON sites in Alaska or on the east coast of North America, which is a region of intense anthropogenic activity (Fig. 1).

European sites

The European region contains eight operational sites (Fig. 2). We also include Izaña, which does not belong to this region but is located very close to it. This region has a good spatial coverage of operational TCCON sites; however, most sites are located near the coast and are thus very sensitive to the Atlantic and Arctic oceans. The maximum footprint sensitivity occurs in western Europe where there is a high density of operational TCCON sites; five sites (Bremen, Garmisch, Karlsruhe, Orléans and Paris) are concentrated within a small area. The sensitivity decreases quite rapidly towards the east and south, and only parts of eastern Europe and northern Africa are covered.

Asia

The footprints of Asian sites mainly span countries bordering the Sea of Japan, i.e. Japan, Korea, the Russian Far East and eastern China. These sites are also able to capture signals from Mongolia, eastern Siberia and South-east Asia. Although the coverage of these sites is relatively small, the main industrial centres in the region are included.

Australia and New Zealand

The footprint sensitivity of TCCON sites in this region covers almost all of Australia. Chevallier et al. (2011) show that TCCON data could constrain flux estimates over Australia equally as well as the existing in situ measurements. Our footprint estimations are, however, more sensitive to the

ocean regions between Australia and New Zealand as well as adjacent coastal areas.

Oceanic sites: Ascension Island and Reunion Island

Ascension Island is in the trade wind belt of the tropical Atlantic, ideally located to measure the South Atlantic marine boundary layer. The south-eastern trade winds, which are almost invariant and are derived from the deep South Atlantic Ocean with little contact with Africa. Surface measurements of CO₂ at Ascension Island are used as a background (Gatti et al., 2010). However, above the trade wind inversion (TWI), at about 1200–2000 m above sea level, the air masses are very different, coming dominantly from tropical Africa and occasionally South America (Swap et al., 1996). The FLEXPART simulation with tracers released at an altitude of 3000 m detected some hotspots in Africa (Fig. 1b). The study of biomass burning in Africa is essential, but lies outside of the scope of this paper.

Reunion Island is situated in the Indian Ocean, about 800 km east of Madagascar. For this site the seasonal trend of wind mainly remains in the easterly sector, so the footprint covers mainly ocean regions. The Reunion Island site is further discussed in Sect. 4.3.2.

3.1.2 Past, future and possible TCCON sites

The footprints of past, future and possible TCCON sites are presented in Fig. 3. The Oxfordshire site enhances the sensitivity of the region, which is already well covered by existing TCCON sites in Europe. The East Trout Lake, Four Corners and Poker Flat sites fill sensitivity gaps in the Canadian boreal forest, the south-western US, northern Mexico and Alaska. Nevertheless, there are no TCCON sites near the Atlantic coast of North America, which is a key region of interest.

In South America, the Manaus site (briefly in operation during 2014 and will operate after reconstruction) was ideally located in central Amazonia. However, meteorological conditions meant that a signal was only detected in a very narrow section towards the east. Observations at this site are more sensitive to anthropogenic activity on the Atlantic coast of South America, compared with the surrounding Amazonian biosphere. Additional use of CO observations will be necessary to isolate the net primary production signal in central Amazonia (Keppel-Aleks et al., 2012). Another site in this region is Paramaribo, located in Suriname, which is part of Caribbean South America. The footprint of the Paramaribo site is narrowly focused towards the Atlantic Ocean due to site location and meteorological conditions as stated above.

Burgo in the northern Philippines extends the Asian footprint southward. The location of the Yekaterinburg site is ideal, as it quite evenly covers a large area of western Russia. The site reduces the gap between the European and Asian

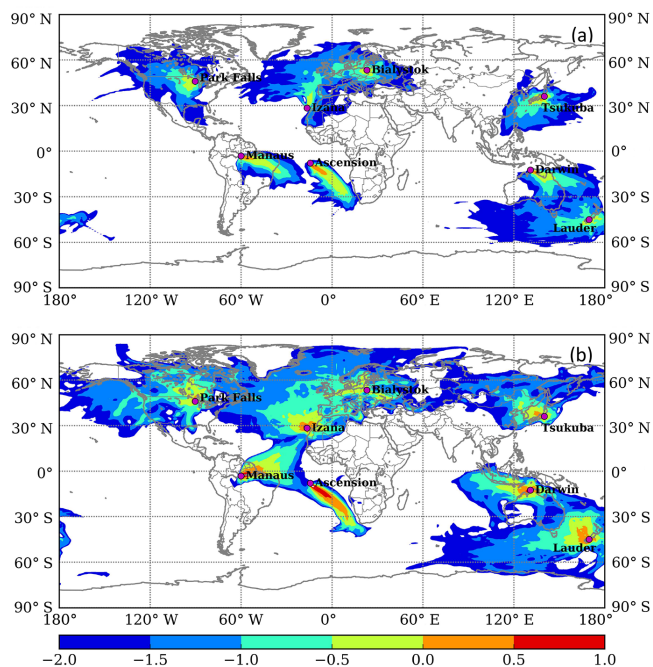


Figure 4. Footprints for different seasons for Ascension Island, Bialystok, Darwin, Izaña, Manaus, Park Falls and Tsukuba, for (a) the summer (June, July and August) of 2010 and (b) the winter (December, January and February) of 2010–2011.

TCCON domains. The Arrival Heights site is located on the Antarctic coast and currently cannot be used for satellite data validation. Given the air circulation near the South Pole, this site can be useful for measuring the background value of XCO₂.

In general, the operational stations cover some regions well (North America, Europe, the Far East, South-east Asia, Australia and New Zealand), and the planned sites will improve this coverage. However, on a global scale there are major gaps that highlight the difficulty in generalising the available data along latitude for bias correction.

The short-term variations in CO₂ in the near surface and free troposphere (< 3000 m) have the same form, but different intensities (Fig. 1b), as a smaller number of tracers from the middle troposphere reached the surface during the simulation time.

Seasonal variability in footprints

Some TCCON stations have strong seasonal variations in their footprint due to changes in wind direction, i.e. Bialystok, Darwin, Izaña, Park Falls and Tsukuba (Fig. 4). For other sites (e.g. Ascension Island and Manaus) the weather conditions are less variable throughout the year. The depth of the PBL changes with season and is thus an important factor that influences the footprint. In winter weak vertical mixing causes the shallow PBL. This leads to enhanced horizontal tracer transport and a wider spatial coverage of the footprints.

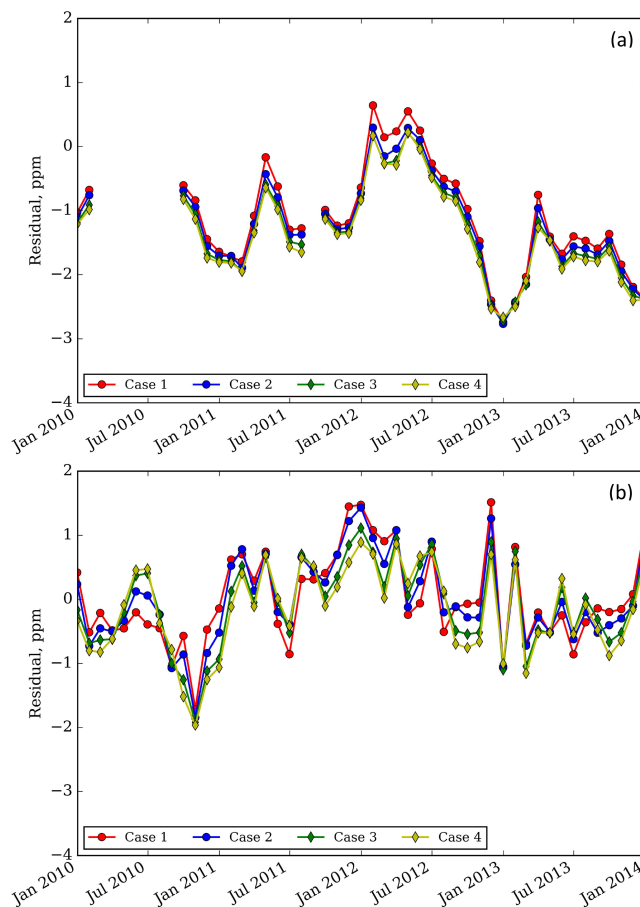


Figure 5. Monthly average residuals of modelled XCO₂ compared with TCCON ground-based FTS for methods C1, C4, C5 and C8, for (a) Darwin and (b) Garmisch.

4 Applying the model-derived footprints to the collocation of XCO₂

In the next two sections we assess the performance of the footprint-based method of collocating TCCON XCO₂ against the NIES model and GOSAT product data sets. The collocation domain size for each site is determined by sensitivity values (ppm (μmol (m² s)⁻¹)⁻¹) with the limits of log₁₀(x) equal to -0.5, -1.0, -1.5 and -2.0 (cases C1–C4). These sensitivity values were selected to approximately correspond to the domain sizes in standard geographical collocation techniques, which have rectangular dimensions of 2.5° × 2.5°, ±5.0° × ±5.0°, ±5.0° × ±10.0° and ±7.5° × ±22.5° (cases C5–C8). Only coincident observations were used, and observations with differences of ≥ 3 ppm were discarded from the comparison. The considered period for comparison is January 2010 and January 2014.

TCCON observations were used from 16 sites: Bialystok, Caltech, Darwin, Eureka, Garmisch, Izaña, Karlsruhe, Lamont, Lauder (125HR), Orléans, Park Falls, Reunion Island, Saga, Sodankylä, Tsukuba (125HR) and Wollongong. These

Table 3. Averaged results of different collocation methods implemented for XCO₂ from NIES TM calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of cells*	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	35	5.33	0.96	0.75	1.01
C2	Footprint limit $\log_{10}(x) = -1.0$	160	5.48	0.96	0.81	0.98
C3	Footprint limit $\log_{10}(x) = -1.5$	507	5.90	0.97	0.85	0.97
C4	Footprint limit $\log_{10}(x) = -2.0$	1071	6.97	0.97	0.88	0.96
C5	Within area of $2.5^\circ \times 2.5^\circ$	1	5.76	0.96	0.76	1.03
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	16	5.36	0.96	0.79	1.00
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	32	5.22	0.96	0.79	0.98
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	108	5.11	0.97	0.80	0.97

* The number of FLEXPART cells with resolution $1.0^\circ \times 1.0^\circ$ is counted for methods based on the footprint (1–4), while for other methods NIES TM cells ($2.5^\circ \times 2.5^\circ$) are used.

Table 4. Averaged results of different collocation methods implemented for XCO₂ from the GOSAT ACOS product calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of observations	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	1190	9.85	0.93	0.65	1.18
C2	Footprint limit $\log_{10}(x) = -1.0$	3046	7.75	0.92	0.61	1.21
C3	Footprint limit $\log_{10}(x) = -1.5$	4880	7.82	0.93	0.62	1.15
C4	Footprint limit $\log_{10}(x) = -2.0$	6016	7.06	0.93	0.64	1.12
C5	Within area of $2.5^\circ \times 2.5^\circ$	976	10.29	0.93	0.81	1.11
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	2042	8.68	0.92	0.67	1.19
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	3111	8.18	0.92	0.65	1.19
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	5002	7.27	0.93	0.64	1.16

observations were obtained from the 2014 release of TCCON data (GGG2014), available from the TCCON Data Archive (<http://tccon.ornl.gov>).

4.1 Collocation of XCO₂ from TCCON and the NIES model

The TCCON and NIES TM data sets are initially compared using a geographical collocation of $2.5^\circ \times 2.5^\circ$, which corresponds to selecting the nearest NIES TM cell (Table 3). The resolution of the model grid is rather coarse, so we observe that the results depend mainly on the size of the collocation area but not on the form. As the size of the collocation area increases, the correlation between XCO₂ from TCCON and NIES TM slightly increases from 0.96 to 0.97 and the standard deviation decreases from 1.1 to 0.96 ppm. This is due to an increase in the number of observations.

There are several reasons for the larger discrepancy (≥ 3 ppm) of GOSAT observations. Systematic errors due to imperfect characterisation of clouds and aerosols dominate the error budget. Other effects, such as spectroscopy errors, pointing errors, imperfect radiometric and spectral charac-

terisation of the instrument are clearly present in retrievals. Additional real-world issues, such as forest canopy effects, partial cloudiness, cloud shadows and plant fluorescence will further increase the retrieval errors (O'Dell et al., 2012). The mean number of discarded coincident observation is about 5–7 %.

For Darwin, Eureka, Izaña, Lauder, Reunion Island, Sodankylä and Wollongong, the residuals between the data sets are small and similar for all methods (see Fig. 5a for Darwin; cases C1, C4, C5 and C8). Here, XCO₂ is under the influence of global long-term variations that are included in the NIES TM. The low sensitivity of the model to local sources does not cause a significant difference between the collocation methods. For the second group (non-operational sites), local sources are essential and even coarse-grid models can capture their signal. As a result, the shape of the collocation area is important (see Fig. 5b for Garmisch; cases C1, C4, C5 and C8).

Table 5. Averaged results of different collocation methods implemented for XCO₂ from the GOSAT NIES product calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of observations	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	1049	10.49	0.89	0.63	1.14
C2	Footprint limit $\log_{10}(x) = -1.0$	2890	11.13	0.92	0.52	1.20
C3	Footprint limit $\log_{10}(x) = -1.5$	4823	9.70	0.92	0.60	1.19
C4	Footprint limit $\log_{10}(x) = -2.0$	5922	8.41	0.92	0.56	1.16
C5	Within area of $2.5^\circ \times 2.5^\circ$	907	11.68	0.89	0.63	1.17
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	1845	10.35	0.91	0.56	1.15
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	2976	10.04	0.93	0.58	1.15
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	4874	9.76	0.92	0.60	1.17

Table 6. Averaged results of different collocation methods implemented for XCO₂ from the GOSAT PPDF product calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of observations	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	357	7.80	0.84	0.50	1.11
C2	Footprint limit $\log_{10}(x) = -1.0$	870	9.07	0.86	0.62	1.12
C3	Footprint limit $\log_{10}(x) = -1.5$	1536	7.81	0.81	0.73	1.16
C4	Footprint limit $\log_{10}(x) = -2.0$	1911	6.46	0.81	0.67	1.17
C5	Within area of $2.5^\circ \times 2.5^\circ$	331	7.02	0.86	0.66	1.02
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	749	7.53	0.85	0.64	1.15
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	1114	8.46	0.83	0.69	1.19
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	1733	7.43	0.86	0.68	1.17

4.2 Collocation of XCO₂ from TCCON and GOSAT products

A comparison of collocation methods was performed for five GOSAT XCO₂ products: NIES v02.11 (Yoshida et al., 2013) and the photon path length probability density function method retrievals (PPDF-S v02.11; Oshchepkov et al., 2013) from the NIES, Japan; the NASA Atmospheric CO₂ Observations from Space retrieval (ACOS B3.4; O'Dell et al., 2012); the Netherlands Institute for Space Research/Karlsruhe Institute of Technology, Germany (RemoTeC v2.11; Butz et al., 2011; Guerlet et al., 2013); and the University of Leicester Full Physics retrieval (UoL-FP v4; Boesch et al., 2011; Cogan et al., 2012). The mean percentage of discarded coincident TCCON–GOSAT observation is around 7–14 %. Results from PPDF and UoL-FP methods are closer to lower and upper limits.

The results of the comparison of eight collocation methods employed for the five GOSAT XCO₂ products are presented in Tables 4–8. Only coincident observations were used, and observations with differences of ≥ 3 ppm were discarded from the comparison. The number of observations se-

lected for collocation between the methods with the smallest areas (C1 and C5) and largest areas (C4 and C8) differs approximately by a factor of 5. There is, however, no clear dependence of the collocation efficiency on the number of observations. The correlation coefficient and standard deviation are within 0.81–0.93 and 1.02–1.22 ppm, respectively, regardless of the method used. Mean bias values are within 0.50–0.87 ppm, with the footprint method typically having a slightly lower bias by 0.02–0.15 ppm and a higher number of collocations. For individual stations, these statistics may lie slightly outside the specified ranges.

4.3 Case study

In this section we demonstrate the developed collocation method for GOSAT observations over the Darwin and Reunion Island TCCON sites.

4.3.1 Darwin site

The Northern Territory of Australia has two distinctive climate zones: the northern and southern zones. The northern zone, including Darwin, has three distinct seasons: the

Table 7. Averaged results of different collocation methods implemented for XCO₂ from the GOSAT RemoTeC product calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of observations	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	795	10.20	0.81	0.71	1.17
C2	Footprint limit $\log_{10}(x) = -1.0$	1898	9.63	0.83	0.66	1.19
C3	Footprint limit $\log_{10}(x) = -1.5$	3212	9.19	0.83	0.61	1.22
C4	Footprint limit $\log_{10}(x) = -2.0$	4091	8.12	0.83	0.59	1.21
C5	Within area of $2.5^\circ \times 2.5^\circ$	769	11.20	0.90	0.87	1.15
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	1491	9.91	0.85	0.63	1.18
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	2325	9.46	0.86	0.70	1.19
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	3818	8.57	0.86	0.64	1.25

Table 8. Averaged results of different collocation methods implemented for XCO₂ from the GOSAT UoL-FP product calculated for 16 TCCON sites.

Case	Method of collocation	Mean number of observations	Mean number of discarded coincident obs. (%)	Mean correlation coefficient	Absolute value of mean bias	Mean standard deviation
C1	Footprint limit $\log_{10}(x) = -0.5$	634	11.04	0.88	0.78	1.31
C2	Footprint limit $\log_{10}(x) = -1.0$	1454	12.78	0.87	0.76	1.34
C3	Footprint limit $\log_{10}(x) = -1.5$	2450	10.88	0.88	0.80	1.28
C4	Footprint limit $\log_{10}(x) = -2.0$	3017	10.22	0.89	0.70	1.23
C5	Within area of $2.5^\circ \times 2.5^\circ$	629	11.90	0.86	0.73	1.33
C6	Within area of $\pm 5.0^\circ \times \pm 5.0^\circ$	1215	13.15	0.88	0.76	1.30
C7	Within area of $\pm 5.0^\circ \times \pm 10.0^\circ$	1852	13.58	0.86	0.74	1.27
C8	Within area of $\pm 7.5^\circ \times \pm 22.5^\circ$	2799	11.93	0.85	0.72	1.25

Table 9. Comparison of collocation methods C4 and C8 using ACOS, NIES, PPDF, RemoTeC and UoL GOSAT products near the Darwin site.

GOSAT Product	Case	Correlation coefficient	Mean bias	Standard deviation	Number of observations
ACOS	C4	0.96	0.36	0.77	36 292
	C8	0.94	0.50	0.90	10 872
NIES	C4	0.94	0.09	0.88	26 652
	C8	0.93	0.13	1.00	6924
PPDF	C4	0.70	0.24	1.02	13 681
	C8	0.64	0.08	1.10	4333
RemoTeC	C4	0.91	0.44	0.95	23 915
	C8	0.89	0.77	1.07	7130
UoL	C4	0.82	0.34	1.17	14 376
	C8	0.86	0.17	1.10	4727

Table 10. Comparison of collocation methods C4 and C8 using ACOS, NIES, RemoTeC and UoL GOSAT products near the Reunion Island site. The PPDF GOSAT product does not include any observations near the Reunion Island site.

GOSAT Product	Case	Correlation coefficient	Mean bias	Standard deviation	Number of observations
ACOS	C4	0.82	0.70	0.83	11 873
	C8	0.83	0.65	0.76	9640
NIES	C4	0.70	0.25	1.07	7720
	C8	0.73	0.45	1.02	6505
RemoTeC	C4	0.51	0.92	1.07	2482
	C8	0.61	1.16	1.04	3414
UoL	C4	0.45	0.75	0.94	860
	C8	0.36	0.71	1.00	2239

dry season (May–September), the build-up season (high humidity, but little rain: October–December) and the wet season, associated with tropical cyclones and monsoon rains (December–April). The average maximum temperature is re-

markably similar all year round. The southern zone is mainly desert with a semi-arid climate and little rain. To the north of Darwin, the territory is bordered by the Timor Sea, the Arafura Sea and the Gulf of Carpentaria. The Northern Territory, therefore, has a pronounced seasonal variability that

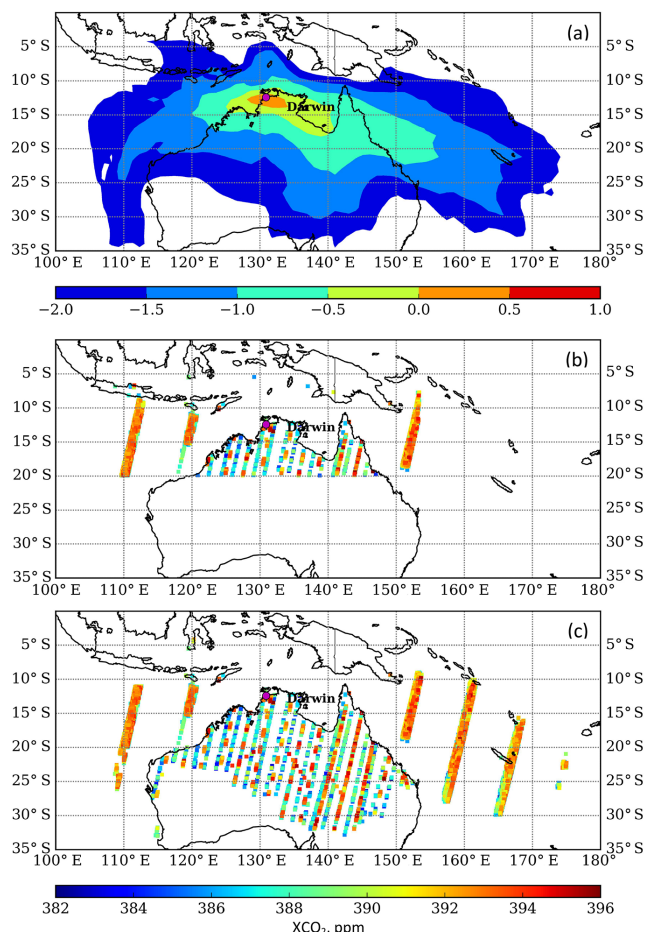


Figure 6. (a) Annual average footprint for the Darwin TCCON observation site; ACOS GOSAT XCO₂ observations selected using (b) the geostatistical method within an area of $\pm 7.5^\circ \times \pm 22.5^\circ$ and (c) the footprint-based method with the limit $\log_{10}(x) = -2.0$.

affects the spatial and temporal distribution of CO₂ and thus the footprint (Figs. 4 and 6a).

Figure 6b and c show the locations of GOSAT observations selected using a geographical method within an area of $\pm 7.5^\circ \times \pm 22.5^\circ$ and a footprint-based method with the limit $\log_{10}(x) = -2.0$. Sizes of selected collocation areas (C4 and C8 methods) are close to ones used in others works (Wunch et al., 2011; Guerlet et al., 2013; Inoue et al., 2013; Reuter et al., 2013; Nguyen et al., 2014).

For ACOS, NIES and RemoTeC GOSAT products the distributions of XCO₂ data sets for the Darwin site are similar and cover an area to the west of Darwin, including ground-based observations from central Australia (Fig. 6c). The comparison of collocation methods shows that the footprint-based method (C4) outperforms the geographical method (C8) for these three GOSAT products (Fig. 7, Table 9), with approximately three times as many observations.

Although currently the UoL GOSAT XCO₂ version 6 includes ocean-glint observations, in this study we use the

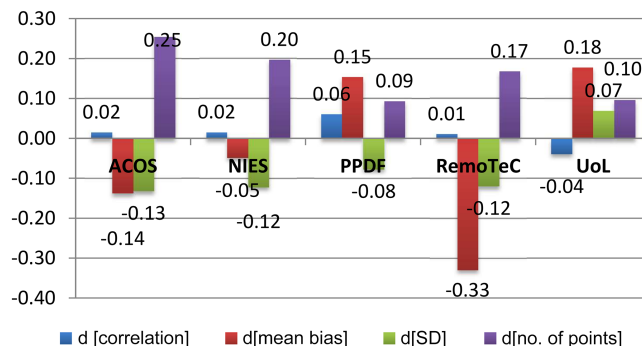


Figure 7. Difference (denoted as $d[]$) in correlation coefficients, mean bias (ppm), SD (ppm) and number of observational points between methods C4 (the collocation domain size is determined by sensitivity values ($\text{ppm}(\mu\text{mol}(\text{m}^2 \text{s})^{-1})^{-1}$) with the limit of $\log_{10}(x)$ equal to -2.0) and C8 (the collocation domain size is rectangular with dimension $\pm 7.5^\circ \times \pm 22.5^\circ$) using ACOS, NIES, PPDF, RemoTeC and UoL GOSAT products near the Darwin site. Please note that the scale of number of observational points is 10^5 .

slightly outdated UoL-FP GOSAT product v4, which has only overland points. In this case the difference between collocation subsets is the observations towards the south over land, which provide a similar distribution to the ACOS product, but without marine observations (Fig. 6b and c). These differences in the covered areas have a significant negative effect on the result (Fig. 7). From that it can be concluded that XCO₂ patterns towards the south over land are rather different from those around Darwin, the sun-glint observation over the ocean are important and must be included into analysis. Thus, XCO₂ at the Darwin site is under the influence of the three different fluxes coming from surrounding land area, central part of Australia and oceanic regions. The oceanic observation over the Coral Sea is quite important, though substantially removed from the station.

4.3.2 Reunion Island site

Reunion Island is a small island east of Madagascar surrounded by the Indian Ocean. The nearest land territory to Reunion Island is Mauritius, located ~ 175 km to the north-west. The meteorological conditions in the region mean that the footprint of the Reunion Island site mostly covers a large area of ocean to the south-east of the island and a small area of northern Madagascar (Fig. 8).

The geographical collocation method does not take into account local conditions. Therefore, despite the fact that the site is predominantly oceanic, the geographical method includes observations made over land in Madagascar and the south-east coast of Africa (Fig. 8b). In contrast, the footprint method takes into account the local meteorology, so observations are predominantly taken from the ocean (Fig. 8c). Since the UoL-FP data set has no observations over the sea, the ob-

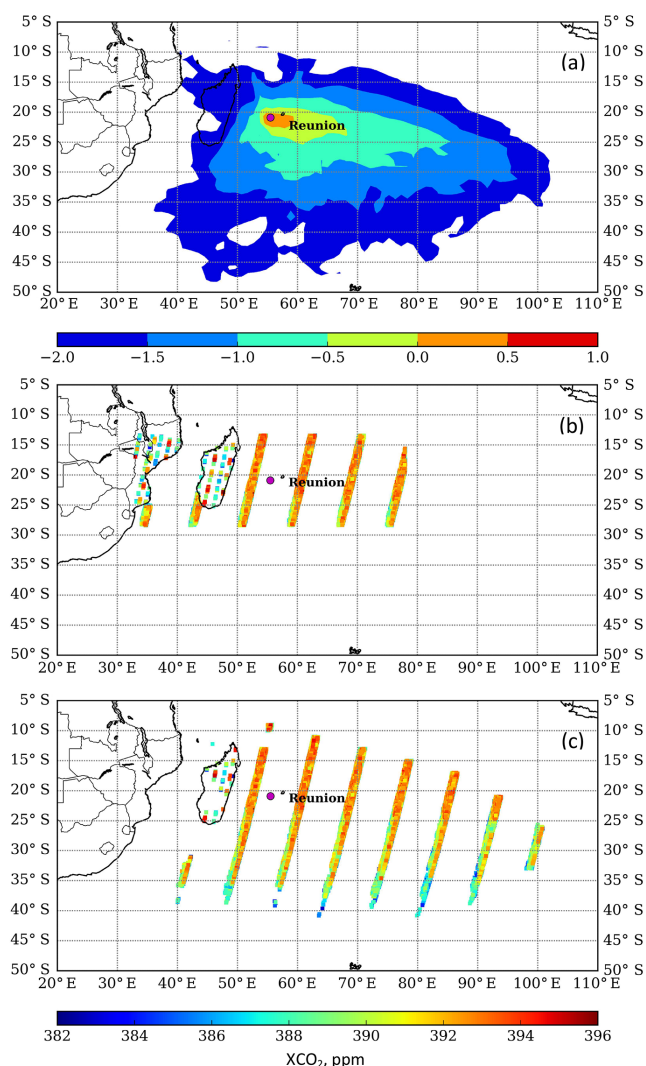


Figure 8. (a) Annual average footprint for the Reunion Island TCCON observation site; ACOS GOSAT XCO₂ observations selected using (b) the geostatistical method within an area of $\pm 7.5^\circ \times \pm 22.5^\circ$ and (c) the footprint-based method with the limit $\log_{10}(x) = -2.0$.

servations for this data set are located only over Madagascar (Fig. 9).

Unlike Darwin, Reunion Island receives clean air from the ocean and thus has very little CO₂ variation. The selection of areas for collocation, therefore, did not reveal any significant advantages of the footprint-based method, with the exception of a slightly smaller bias for the NIES and RemoTeC products (Fig. 10, Table 10). The comparison of the UoL-FP product for method C4 and method C8 shows that the XCO₂ cycles over Madagascar and the eastern coast of Africa are quite different (Fig. 10). This highlights that the exclusion of marine observations leads to poor results over marine-based TCCON sites.

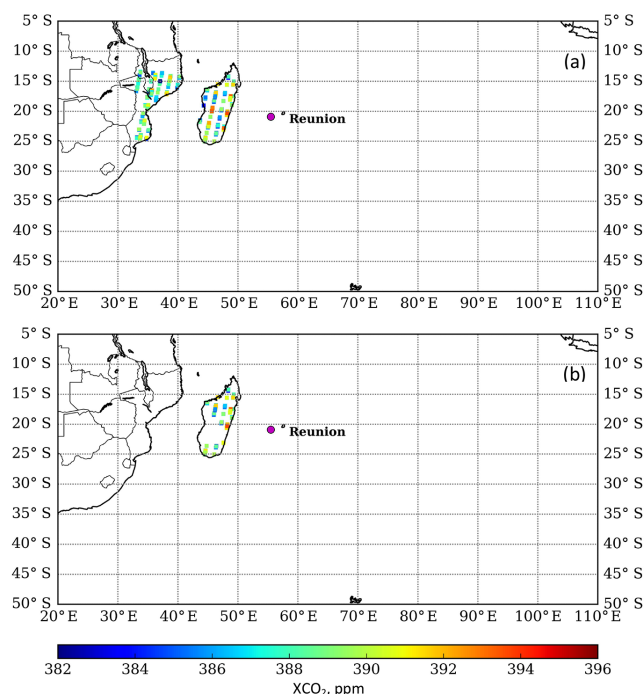


Figure 9. UoL-FP GOSAT XCO₂ observations selected using (a) the geostatistical method within an area of $\pm 7.5^\circ \times \pm 22.5^\circ$ and (b) the footprint-based method with the limit $\log_{10}(x) = -2.0$.

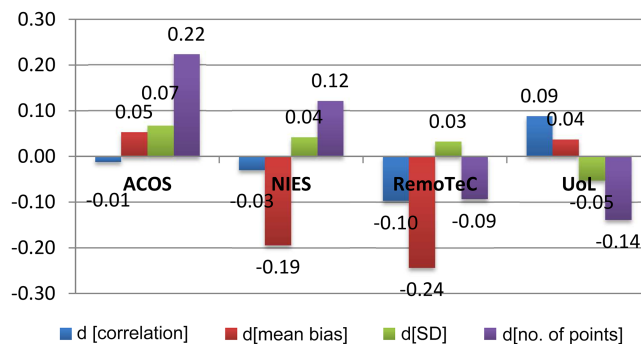


Figure 10. Difference (denoted as $d[\]$) in correlation coefficients, mean bias (ppm), SD (ppm) and number of observational points between methods C4 (the collocation domain size is determined by sensitivity values $(\text{ppm}(\mu\text{mol}(\text{m}^2\text{s})^{-1})^{-1})$ with the limit of $\log_{10}(x)$ equal to -2.0) and C8 (the collocation domain size is rectangular with dimension $\pm 7.5^\circ \times \pm 22.5^\circ$) using ACOS, NIES, RemoTeC and UoL GOSAT products near the Reunion Island site. Please note scale of number of observational points is 10^4 .

A comparison of TCCON data and NIES model results for Darwin and Reunion shows that XCO₂ for these sites is controlled mainly by large-scale changes. However, analysis of GOSAT products emphasises that the influence of local fluxes is also important (Liu et al., 2015). The geographical method of collocation assumes a fairly even distribution of GOSAT observations near TCCON sites, while the cal-

culated footprints have strongly curved shapes and an uneven distribution. We therefore expect the proposed footprint method to be useful for other sites with rather curved and non-uniform footprints, such as the Ascension Island and Manaus sites.

5 Summary

We have developed a method for assessing the footprints of short-term XCO₂ variations observed by TCCON ground-based FTS sites. The method is based on 1-week FLEXPART backward trajectory simulations that are initiated at an altitude of 1 km (the upper border of the PBL) in the afternoon using the vertical CO₂ distribution calculated by the NIES transport model.

We applied this method to estimate footprints of the operational, past, future and possible TCCON sites, and revealed some basic patterns. Most sites located near coastal regions are strongly influenced by ocean regions; thus, there is a large seasonal variability in footprints for Białystok, Darwin, Izaña, Park Falls and Tsukuba. The Ascension Island, Manaus and Reunion Island sites have very narrow footprints that show small seasonal variations.

We proposed the footprint-based method for the collocation of satellite observations with TCCON sites, and assessed the performance of the method using the NIES model and GOSAT product data sets. The collocation footprint area is determined by yearly averaged sensitivity values with limits of $\log_{10}(x)$ equals -0.5 , -1.0 , -1.5 and -2.0 . These were selected to approximately correspond to the areas of standard geographical collocation techniques that have rectangular shapes of $2.5^\circ \times 2.5^\circ$, $\pm 5.0^\circ \times \pm 5.0^\circ$, $\pm 5.0^\circ \times \pm 10.0^\circ$ and $\pm 7.5^\circ \times \pm 22.5^\circ$, respectively. A comparison of the proposed method with the geographical method showed similar but smaller biases for a subset of 16 stations for the period from January 2009 to January 2014. Case studies of the Darwin and Reunion Island TCCON sites revealed that the footprint has a very different collocation area to that of the geographical method, especially near marine coast.

The geographical collocation (and other similar methods) is based on tracking long-term trends of tracers (i.e. derived from global model calculations) and is therefore less sensitive to the influence of local sources. This approach shows good performance for current precision of satellite XCO₂ retrievals, but it has its limitations and works up to a certain accuracy threshold. Given that the GOSAT XCO₂ products are sensitive to local sources, the proposed footprint method is promising and requires further fine-tuning. The potential for further improvement includes moving from gross annual averaging to more accurate seasonal or monthly averaging. In addition, it is possible to study the sensitivity of XCO₂ observations using the adjoint of the global Eulerian–Lagrangian coupled atmospheric transport model (Belikov et al., 2016),

which can resolve long-term, synoptic and hourly variation patterns.

We believe, however, that the footprint analysis should be considered important in the appraisal of new TCCON sites, along with assessments of the number of cloudless days, the surrounding landscape and the reflectivity of the earth's surface.

6 Data availability

The data sets are available at <ftp://tcccon.ornl.gov/2014Public/documentation/> (Wunch et al., 2015).

The JRA-25/JCDAS meteorological data sets used in the simulations were provided by the Japan Meteorological Agency. The computational resources were provided by NIES. This study was performed by order of the Ministry for Education and Science of the Russian Federation No. 5.628.2014/K and was supported by The Tomsk State University Academic D. I. Mendeleev Fund Program in 2014–2015 and by the GRENE Arctic project.

TCCON data were obtained from the TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center (CDIAC) at Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, <http://tcccon.ornl.gov>. The Ascension Island site has been funded by the Max Planck Society. The Bremen, Białystok and Orléans TCCON sites are funded by the EU projects InGOS and ICOS-INWIRE, and by the Senate of Bremen. The Darwin and Wollongong TCCON sites are funded by NASA grants NAG5-12247 and NNG05-GD07G, and Australian Research Council grants DP140101552, DP110103118, DP0879468, LE0668470 and LP0562346. We are grateful to the DOE ARM programme for technical support at the Darwin TCCON site. Nicholas Deutscher was supported by an Australian Research Council fellowship, DE140100178.

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